

Editorial

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Preface: Numerical Analysis of Fractional Differential Equations

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Fractional PDEs, which involve a fractional-order derivative in time or/and space and more generally non-local derivatives (e.g., fractional Laplacian), have been established as extremely powerful modeling tools. Fractional PDEs can adequately describe transport processes collectively known as anomalous diffusion, where the mean squared displacement grows sublinearly/superlinearly with the time, as opposed to the linear growth for normal diffusion. The spectrum of their practical applications is very broad and spans many diverse disciplines, e.g., subsurface flow, thermal diffusion in fractal domains, and dynamics of protein molecules.

Compared with mathematical models describing normal diffusion, nonlocal models pose substantial challenges to both their rigorous analysis and their numerical treatment. Hence, the development of reliable and efficient numerical schemes and their analysis is of significant theoretical and practical interest. In the last two decades, intensive research has been carried out in this area.

This special issue consists of fourteen invited contributions (four in the current issue, and the remaining ten in issue 18(1)) on novel numerical methods for nonlocal models and their mathematical analysis. These papers cover a broad range of topics including construction of computational schemes, stability and error analysis, and testing and numerical simulations. Below we briefly describe the content of the special issue.

The papers [2, 14, 17, 18, 27, 35] deal with the time fractional diffusion problem, which involves a fractional-order derivative of either Riemann–Liouville or Caputo type in time of order $\alpha \in (0, 1)$. It is frequently employed to describe subdiffusion processes, and hence also known as the subdiffusion equation in the literature. This model can be viewed as the macroscopic counterpart of continuous time random walk.

The solution to the subdiffusion problem usually contains a weak singularity at time $t = 0$, even for smooth problem data. Thus spectral methods using polynomials generally do not work well. One promising idea is to use nonpolynomial functions [9]. The paper [17] proposes two spectral methods for the subdiffusion equation by approximating the solution by Müntz polynomials, based on Galerkin formulation and Petrov–Galerkin formulation, respectively, and shows that both methods are exponentially convergent for general source terms, for which the exact solution has very limited regularity.

Due to the limited smoothing property of the solution operator, many time stepping schemes are only first-order accurate in time, if implemented straightforwardly. The paper [35] studies a time stepping scheme, which can be derived via either Diethelm's method [12] or piecewise constant discontinuous Galerkin method [30]. Just as expected, a direct implementation of the method has only an $O(\tau)$ rate, with τ being the time step size. The authors propose an interesting corrected variant of the scheme, which modifies only the first step of the scheme while improves the convergence rate to $O(\tau^{1+\alpha})$, in a manner similar to the works [10, 20, 21].

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The L1 scheme [29] is one of the most popular schemes for discretizing the Caputo derivative, and there have been several error analyses under different conditions [19, 24, 33]. The paper [16] revisits the error analysis of the L1 scheme for the subdiffusion model with a convection term, and shows that the convergence in the maximum norm on any subdomain bounded away from $t = 0$ is higher than the rate over the entire space-time domain.

Space-time formulations have received increasing attention for parabolic problems, and recently also for the subdiffusion problem [28, 36]. The paper [14] develops a novel space-time Petrov–Galerkin formulation with different trial and test spaces for the subdiffusion model, and establishes its inf-sup condition (and thus well-posedness of the formulation). Together with a tensor-product trial space using fractional piecewise constant functions in time and conforming linear FEM space in space, it leads to a Petrov–Galerkin FEM formulation. The work provides the well-posedness of the discrete problem and error bounds in both energy and L^2 norms for the FEM solution.

Most studies on the subdiffusion problem are for bounded domains. The paper [27] presents a numerical method for the time-fractional Schrödinger equation on an unbounded domain, by constructing artificial boundary conditions for a truncated domain and applying the L1 scheme accelerated by sum-of-exponentials approximation. The authors give a stability analysis of the truncated problem and the numerical schemes.

The usual subdiffusion equation involves only one single Caputo/Riemann–Liouville derivative, and more complex derivatives, e.g., multi-term, distributed-order and variable-order, can be employed to model more realistic physical processes. The paper [2] presents a difference scheme for the Caputo-type derivative with a generalized memory kernel analogous to the L1 scheme. The author applies it to approximate a generalized subdiffusion equation, and discusses its stability and convergence rate in the discrete L^2 norm.

The works [3, 5, 11, 15, 18, 32, 34, 37] study the space fractional model or time-space fractional models. Such models arise in the mathematical modeling of superdiffusion processes, and can be viewed as the macroscopic counterpart of Lévy process. There are a variety of definitions of space fractional differential operators: Riesz fractional derivative, fractional Laplacian and nonlocal models, and they are generally not equivalent to each other on bounded domains [13, 26].

One unceasing theme in applied mathematics is to establish the connections between microscopic and macroscopic models. The paper [11] introduces a nonlocal convection-superdiffusion model for the master equation of Markov jump processes on bounded domains, and shows the well-posedness of the nonlocal steady and unsteady state master equations in a weak sense under minimal assumptions on the model parameters. The authors prove that the nonlocal operator is the generator of finite-range nonsymmetric jump processes and the generators of finite and infinite activity Lévy and Lévy-type jump processes are special cases of the nonlocal operator.

The fractional derivative/fractional Laplacian over the real line can be viewed as the infinitesimal generator of α -stable Lévy motions [25]. The paper [18] presents several finite difference methods for 1D asymmetric infinitesimal generator, by viewing it as a multiplier in the spectral space. These methods take the form of a discrete convolution, with the weights chosen to approximate the exact multiplier in the spectral space. The authors provide detailed discussions on their accuracy and advantages/disadvantages.

On bounded domains, the fractional power of an elliptic operator is a popular choice for space fractional derivative, and can be evaluated efficiently via Dunford–Taylor integral together with suitable quadrature rules [6]. The paper [5] presents a numerical scheme for a space-time fractional parabolic equation, with a Caputo derivative in time and a fractional-power elliptic operator in space. The authors develop semi-discrete methods based on finite element approximation to the underlying (non-fractional) spatial operator and fully discrete methods based on a sinc quadrature technique for the Dunford–Taylor integral of the discrete operator, and give error estimates for the approximations.

The paper [34] studies the finite element approximation together with a standard two-level scheme in time for a parabolic equation with the fractional power of a second-order elliptic operator in space. For the practical implementation, the author discusses Padé-type approximations, inspired by special quadrature formulas for Dunford–Taylor integral of the fractional elliptic operator [1], for both explicit and implicit schemes.

Eigenvalue problems with a fractional derivative exhibit many distinct features when compared with the classical Sturm–Liouville problem, and require new computational techniques [22]. The paper [15] presents an algorithm for eigenvalue problems for the fractional Jacobi-type ODE, using piecewise approximation of the coefficients of differential equation and recursion, which gives rise to a sequence of decoupled linear BVPs. Numerically the approach exhibits a super-exponential convergence rate.

Optimal control problems and inverse problems for fractional-order models have received increasing attention due to their practical relevance [23]. The paper [32] considers an optimal control problem for fractional diffusion with a nondifferentiable cost functional and control constraint. The authors give existence, uniqueness and regularity results and first-order optimality conditions, and develop a solver via Caffarelli–Silvestre extension [7, 31]. Further, they propose a fully discrete scheme with piecewise constant functions for the control and first-degree tensor product finite elements for the state, and derive quasi-optimal a priori error estimates for the control and state variables.

The list of applications of fractional differential operators is ever increasing. The paper [3] explores the application of in image processing and phase field models, where jumps across subsets and sharp transitions across interfaces are of interest. The authors analyze a spectral method for the solution of some model problems, and numerically illustrate their features.

The Bloch–Torrey equation is one canonical model in magnetic resonance imaging. The paper [37] presents a difference scheme for 1D space-time fractional Bloch–Torrey equation, with the weighted and shifted Grünwald–Letnikov difference for the Caputo derivative in time [4, 8], and fractional central difference for the Riesz fractional derivative in space. The authors show the unique solvability, unconditional stability and convergence rate of the scheme by an energy method.

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References

- [1] L. Aceto and P. Novati, Rational approximation to the fractional Laplacian operator in reaction-diffusion problems, *SIAM J. Sci. Comput.* **39** (2017), no. 1, A214–A228.
- [2] A. Alikhanov, A time-fractional diffusion equation with generalized memory kernel in differential and difference settings with smooth solutions, *Comput. Methods Appl. Math.* **17** (2017), no. 4, 647–660.
- [3] H. Antil and S. Bartels, Spectral approximation of fractional PDEs in image processing and phase field modeling, *Comput. Methods Appl. Math.* **17** (2017), no. 4, 661–678.
- [4] B. Baeumer, M. Kovács and H. Sankaranarayanan, Higher order Grünwald approximations of fractional derivatives and fractional powers of operators, *Trans. Amer. Math. Soc.* **367** (2015), no. 2, 813–834.
- [5] A. Bonito, W. Lei and J. E. Pasciak, Numerical approximation of space-time fractional parabolic equations, *Comput. Methods Appl. Math.* **17** (2017), no. 4, 679–705.
- [6] A. Bonito and J. E. Pasciak, Numerical approximation of fractional powers of elliptic operators, *Math. Comp.* **84** (2015), no. 295, 2083–2110.
- [7] L. Caffarelli and L. Silvestre, An extension problem related to the fractional Laplacian, *Comm. Partial Differential Equations* **32** (2007), no. 7–9, 1245–1260.
- [8] M. Chen and W. Deng, Fourth order accurate scheme for the space fractional diffusion equations, *SIAM J. Numer. Anal.* **52** (2014), no. 3, 1418–1438.
- [9] S. Chen, J. Shen and L.-L. Wang, Generalized Jacobi functions and their applications to fractional differential equations, *Math. Comp.* **85** (2016), no. 300, 1603–1638.
- [10] E. Cuesta, C. Lubich and C. Palencia, Convolution quadrature time discretization of fractional diffusion-wave equations, *Math. Comp.* **75** (2006), no. 254, 673–696.
- [11] M. D’Elia, Q. Du, M. Gunzburger and R. Lehoucq, Nonlocal convection-diffusion problems on bounded domains and finite-range jump processes, *Comput. Methods Appl. Math.* **17** (2017), no. 4, 707–722.
- [12] K. Diethelm, An algorithm for the numerical solution of differential equations of fractional order, *Electron. Trans. Numer. Anal.* **5** (1997), 1–6.

- [13] Q. Du, M. Gunzburger, R. B. Lehoucq and K. Zhou, Analysis and approximation of nonlocal diffusion problems with volume constraints, *SIAM Rev.* **54** (2012), no. 4, 667–696.
- [14] B. Duan, B. Jin, R. Lazarov, J. Pasciak and Z. Zhou, Space-time Petrov–Galerkin FEM for fractional diffusion problems, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [15] I. P. Gavriluk, V. Makarov and N. Romaniuk, Super-exponentially convergent parallel algorithm for a fractional eigenvalue problem of Jacobi-type, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [16] J. L. Gracia, E. O’Riordan and M. Stynes, Convergence in positive time for a finite difference method applied to a fractional convection-diffusion equation, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [17] D. Hou, M. T. Hasan and C. Xu, Müntz spectral methods for the time-fractional diffusion equation, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [18] Y. Huang and X. Wang, Finite difference methods for the generator of 1D asymmetric alpha-stable Lévy motions, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [19] B. Jin, R. Lazarov and Z. Zhou, An analysis of the L1 scheme for the subdiffusion equation with nonsmooth data, *IMA J. Numer. Anal.* **36** (2016), no. 1, 197–221.
- [20] B. Jin, R. Lazarov and Z. Zhou, Two fully discrete schemes for fractional diffusion and diffusion-wave equations with nonsmooth data, *SIAM J. Sci. Comput.* **38** (2016), no. 1, A146–A170.
- [21] B. Jin, B. Li and Z. Zhou, Correction of high-order BDF convolution quadrature for fractional evolution equations, preprint (2017), <https://arxiv.org/abs/1703.08808>.
- [22] B. Jin and W. Rundell, An inverse Sturm–Liouville problem with a fractional derivative, *J. Comput. Phys.* **231** (2012), no. 14, 4954–4966.
- [23] B. Jin and W. Rundell, A tutorial on inverse problems for anomalous diffusion processes, *Inverse Problems* **31** (2015), no. 3, Article ID 035003.
- [24] B. Jin and Z. Zhou, An analysis of Galerkin proper orthogonal decomposition for subdiffusion, *ESAIM Math. Model. Numer. Anal.* **51** (2017), no. 1, 89–113.
- [25] V. N. Kolokoltsov, *Markov Processes, Semigroups and Generators*, De Gruyter Stud. Math. 38, Walter de Gruyter, Berlin, 2011.
- [26] M. Kwaśnicki, Ten equivalent definitions of the fractional Laplace operator, *Fract. Calc. Appl. Anal.* **20** (2017), no. 1, 7–51.
- [27] D. Li, J. Zhang and Z. Zhang, The numerical computation of the time fractional Schrödinger equation on an unbounded domain, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [28] X. Li and C. Xu, A space-time spectral method for the time fractional diffusion equation, *SIAM J. Numer. Anal.* **47** (2009), no. 3, 2108–2131.
- [29] Y. Lin and C. Xu, Finite difference/spectral approximations for the time-fractional diffusion equation, *J. Comput. Phys.* **225** (2007), no. 2, 1533–1552.
- [30] W. McLean and K. Mustapha, Time-stepping error bounds for fractional diffusion problems with non-smooth initial data, *J. Comput. Phys.* **293** (2015), 201–217.
- [31] R. H. Nochetto, E. Otárola and A. J. Salgado, A PDE approach to fractional diffusion in general domains: A priori error analysis, *Found. Comput. Math.* **15** (2015), no. 3, 733–791.
- [32] E. Otárola and A. J. Salgado, Sparse optimal control for fractional diffusion, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [33] M. Stynes, E. O’Riordan and J. L. Gracia, Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation, *SIAM J. Numer. Anal.* **55** (2017), no. 2, 1057–1079.
- [34] P. Vabishchevich, Numerical solution of time-dependent problems with fractional power elliptic operator, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [35] Y. Yang, Y. Yan and N. J. Ford, Some time stepping methods for fractional diffusion problems with nonsmooth data, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.
- [36] M. Zayernouri, M. Ainsworth and G. E. Karniadakis, A unified Petrov–Galerkin spectral method for fractional PDEs, *Comput. Methods Appl. Mech. Engrg.* **283** (2015), 1545–1569.
- [37] Y. Zhu and Z.-Z. Sun, A high-order difference scheme for the space and time fractional Bloch–Torrey equation, *Comput. Methods Appl. Math.* **18** (2018), no. 1, to appear.